



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:17 pm BST

PDB ID : 4JX6
Title : Structure of the carboxyl transferase domain Y628A from *Rhizobium etli* pyruvate carboxylase with pyruvate
Authors : Lietzan, A.D.; St Maurice, M.
Deposited on : 2013-03-27
Resolution : 2.78 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

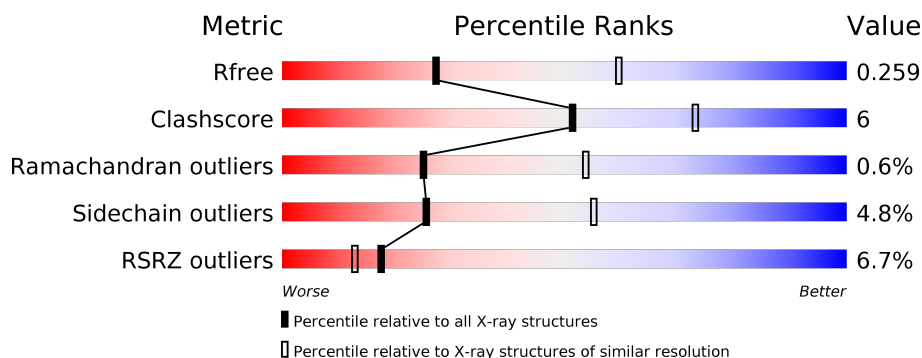
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	632	<div> <div> <div></div> <div>84%</div> <div>10%</div> <div>6%</div> </div> <div> <div>6%</div> <div>81%</div> <div>13%</div> <div>6%</div> </div> </div>
1	B	632	<div> <div>8%</div> <div>77%</div> <div>14%</div> <div>7%</div> </div> <div> <div>10%</div> <div>75%</div> <div>16%</div> <div>8%</div> </div>
1	C	632	
1	D	632	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17344 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	1	0
			4456	2841	739	853	23			
1	B	593	Total	C	N	O	S	0	0	0
			4342	2745	729	846	22			
1	C	588	Total	C	N	O	S	0	1	0
			4247	2691	712	822	22			
1	D	584	Total	C	N	O	S	0	0	0
			4213	2665	706	820	22			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	436	MET	-	EXPRESSION TAG	UNP Q2K340
A	437	GLY	-	EXPRESSION TAG	UNP Q2K340
A	438	SER	-	EXPRESSION TAG	UNP Q2K340
A	439	SER	-	EXPRESSION TAG	UNP Q2K340
A	440	HIS	-	EXPRESSION TAG	UNP Q2K340
A	441	HIS	-	EXPRESSION TAG	UNP Q2K340
A	442	HIS	-	EXPRESSION TAG	UNP Q2K340
A	443	HIS	-	EXPRESSION TAG	UNP Q2K340
A	444	HIS	-	EXPRESSION TAG	UNP Q2K340
A	445	HIS	-	EXPRESSION TAG	UNP Q2K340
A	446	HIS	-	EXPRESSION TAG	UNP Q2K340
A	447	HIS	-	EXPRESSION TAG	UNP Q2K340
A	448	ASP	-	EXPRESSION TAG	UNP Q2K340
A	449	TYR	-	EXPRESSION TAG	UNP Q2K340
A	450	ASP	-	EXPRESSION TAG	UNP Q2K340
A	451	ILE	-	EXPRESSION TAG	UNP Q2K340
A	452	PRO	-	EXPRESSION TAG	UNP Q2K340
A	453	THR	-	EXPRESSION TAG	UNP Q2K340
A	454	SER	-	EXPRESSION TAG	UNP Q2K340
A	455	GLU	-	EXPRESSION TAG	UNP Q2K340
A	456	ASN	-	EXPRESSION TAG	UNP Q2K340

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	457	LEU	-	EXPRESSION TAG	UNP Q2K340
A	458	TYR	-	EXPRESSION TAG	UNP Q2K340
A	459	PHE	-	EXPRESSION TAG	UNP Q2K340
A	460	GLN	-	EXPRESSION TAG	UNP Q2K340
A	461	GLY	-	EXPRESSION TAG	UNP Q2K340
A	462	LEU	-	EXPRESSION TAG	UNP Q2K340
A	463	LEU	-	EXPRESSION TAG	UNP Q2K340
A	464	HIS	-	EXPRESSION TAG	UNP Q2K340
A	628	ALA	TYR	ENGINEERED MUTATION	UNP Q2K340
B	436	MET	-	EXPRESSION TAG	UNP Q2K340
B	437	GLY	-	EXPRESSION TAG	UNP Q2K340
B	438	SER	-	EXPRESSION TAG	UNP Q2K340
B	439	SER	-	EXPRESSION TAG	UNP Q2K340
B	440	HIS	-	EXPRESSION TAG	UNP Q2K340
B	441	HIS	-	EXPRESSION TAG	UNP Q2K340
B	442	HIS	-	EXPRESSION TAG	UNP Q2K340
B	443	HIS	-	EXPRESSION TAG	UNP Q2K340
B	444	HIS	-	EXPRESSION TAG	UNP Q2K340
B	445	HIS	-	EXPRESSION TAG	UNP Q2K340
B	446	HIS	-	EXPRESSION TAG	UNP Q2K340
B	447	HIS	-	EXPRESSION TAG	UNP Q2K340
B	448	ASP	-	EXPRESSION TAG	UNP Q2K340
B	449	TYR	-	EXPRESSION TAG	UNP Q2K340
B	450	ASP	-	EXPRESSION TAG	UNP Q2K340
B	451	ILE	-	EXPRESSION TAG	UNP Q2K340
B	452	PRO	-	EXPRESSION TAG	UNP Q2K340
B	453	THR	-	EXPRESSION TAG	UNP Q2K340
B	454	SER	-	EXPRESSION TAG	UNP Q2K340
B	455	GLU	-	EXPRESSION TAG	UNP Q2K340
B	456	ASN	-	EXPRESSION TAG	UNP Q2K340
B	457	LEU	-	EXPRESSION TAG	UNP Q2K340
B	458	TYR	-	EXPRESSION TAG	UNP Q2K340
B	459	PHE	-	EXPRESSION TAG	UNP Q2K340
B	460	GLN	-	EXPRESSION TAG	UNP Q2K340
B	461	GLY	-	EXPRESSION TAG	UNP Q2K340
B	462	LEU	-	EXPRESSION TAG	UNP Q2K340
B	463	LEU	-	EXPRESSION TAG	UNP Q2K340
B	464	HIS	-	EXPRESSION TAG	UNP Q2K340
B	628	ALA	TYR	ENGINEERED MUTATION	UNP Q2K340
C	436	MET	-	EXPRESSION TAG	UNP Q2K340
C	437	GLY	-	EXPRESSION TAG	UNP Q2K340
C	438	SER	-	EXPRESSION TAG	UNP Q2K340

Continued on next page...

Continued from previous page...

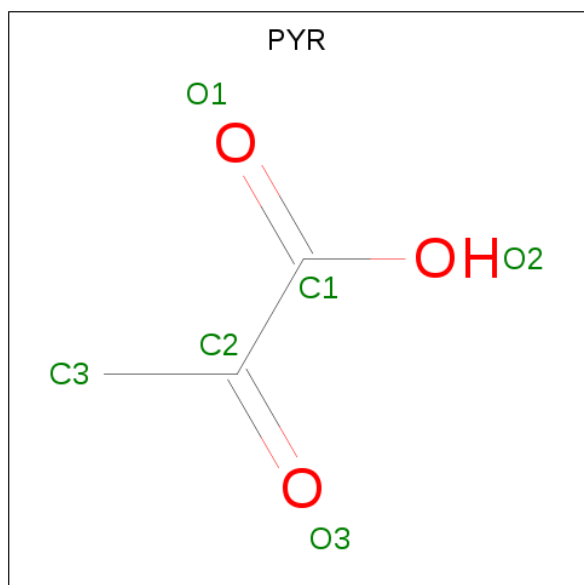
Chain	Residue	Modelled	Actual	Comment	Reference
C	439	SER	-	EXPRESSION TAG	UNP Q2K340
C	440	HIS	-	EXPRESSION TAG	UNP Q2K340
C	441	HIS	-	EXPRESSION TAG	UNP Q2K340
C	442	HIS	-	EXPRESSION TAG	UNP Q2K340
C	443	HIS	-	EXPRESSION TAG	UNP Q2K340
C	444	HIS	-	EXPRESSION TAG	UNP Q2K340
C	445	HIS	-	EXPRESSION TAG	UNP Q2K340
C	446	HIS	-	EXPRESSION TAG	UNP Q2K340
C	447	HIS	-	EXPRESSION TAG	UNP Q2K340
C	448	ASP	-	EXPRESSION TAG	UNP Q2K340
C	449	TYR	-	EXPRESSION TAG	UNP Q2K340
C	450	ASP	-	EXPRESSION TAG	UNP Q2K340
C	451	ILE	-	EXPRESSION TAG	UNP Q2K340
C	452	PRO	-	EXPRESSION TAG	UNP Q2K340
C	453	THR	-	EXPRESSION TAG	UNP Q2K340
C	454	SER	-	EXPRESSION TAG	UNP Q2K340
C	455	GLU	-	EXPRESSION TAG	UNP Q2K340
C	456	ASN	-	EXPRESSION TAG	UNP Q2K340
C	457	LEU	-	EXPRESSION TAG	UNP Q2K340
C	458	TYR	-	EXPRESSION TAG	UNP Q2K340
C	459	PHE	-	EXPRESSION TAG	UNP Q2K340
C	460	GLN	-	EXPRESSION TAG	UNP Q2K340
C	461	GLY	-	EXPRESSION TAG	UNP Q2K340
C	462	LEU	-	EXPRESSION TAG	UNP Q2K340
C	463	LEU	-	EXPRESSION TAG	UNP Q2K340
C	464	HIS	-	EXPRESSION TAG	UNP Q2K340
C	628	ALA	TYR	ENGINEERED MUTATION	UNP Q2K340
D	436	MET	-	EXPRESSION TAG	UNP Q2K340
D	437	GLY	-	EXPRESSION TAG	UNP Q2K340
D	438	SER	-	EXPRESSION TAG	UNP Q2K340
D	439	SER	-	EXPRESSION TAG	UNP Q2K340
D	440	HIS	-	EXPRESSION TAG	UNP Q2K340
D	441	HIS	-	EXPRESSION TAG	UNP Q2K340
D	442	HIS	-	EXPRESSION TAG	UNP Q2K340
D	443	HIS	-	EXPRESSION TAG	UNP Q2K340
D	444	HIS	-	EXPRESSION TAG	UNP Q2K340
D	445	HIS	-	EXPRESSION TAG	UNP Q2K340
D	446	HIS	-	EXPRESSION TAG	UNP Q2K340
D	447	HIS	-	EXPRESSION TAG	UNP Q2K340
D	448	ASP	-	EXPRESSION TAG	UNP Q2K340
D	449	TYR	-	EXPRESSION TAG	UNP Q2K340
D	450	ASP	-	EXPRESSION TAG	UNP Q2K340

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	451	ILE	-	EXPRESSION TAG	UNP Q2K340
D	452	PRO	-	EXPRESSION TAG	UNP Q2K340
D	453	THR	-	EXPRESSION TAG	UNP Q2K340
D	454	SER	-	EXPRESSION TAG	UNP Q2K340
D	455	GLU	-	EXPRESSION TAG	UNP Q2K340
D	456	ASN	-	EXPRESSION TAG	UNP Q2K340
D	457	LEU	-	EXPRESSION TAG	UNP Q2K340
D	458	TYR	-	EXPRESSION TAG	UNP Q2K340
D	459	PHE	-	EXPRESSION TAG	UNP Q2K340
D	460	GLN	-	EXPRESSION TAG	UNP Q2K340
D	461	GLY	-	EXPRESSION TAG	UNP Q2K340
D	462	LEU	-	EXPRESSION TAG	UNP Q2K340
D	463	LEU	-	EXPRESSION TAG	UNP Q2K340
D	464	HIS	-	EXPRESSION TAG	UNP Q2K340
D	628	ALA	TYR	ENGINEERED MUTATION	UNP Q2K340

- Molecule 2 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

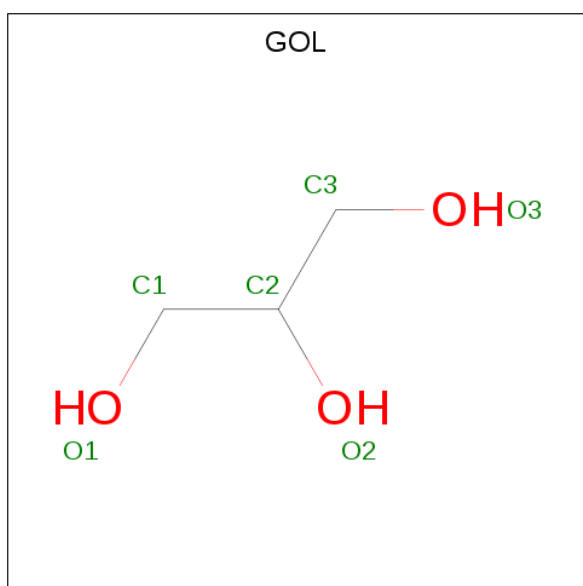
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		

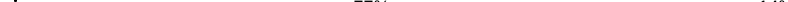
- Molecule 6 is water.

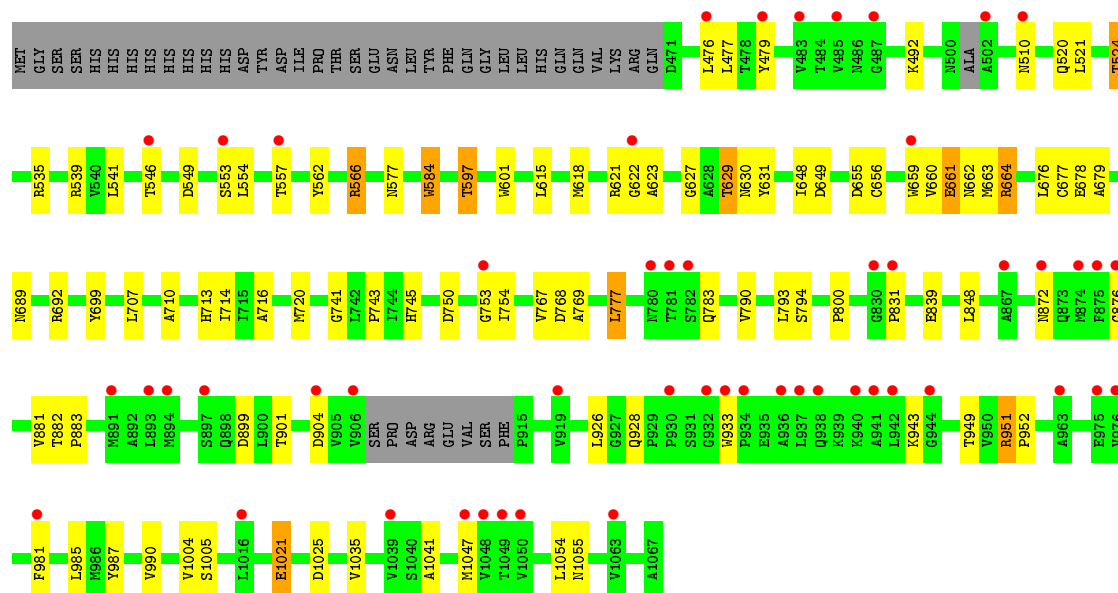
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	28	Total 28	O 28	0	0
6	B	12	Total 12	O 12	0	0
6	C	12	Total 12	O 12	0	0
6	D	8	Total 8	O 8	0	0

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

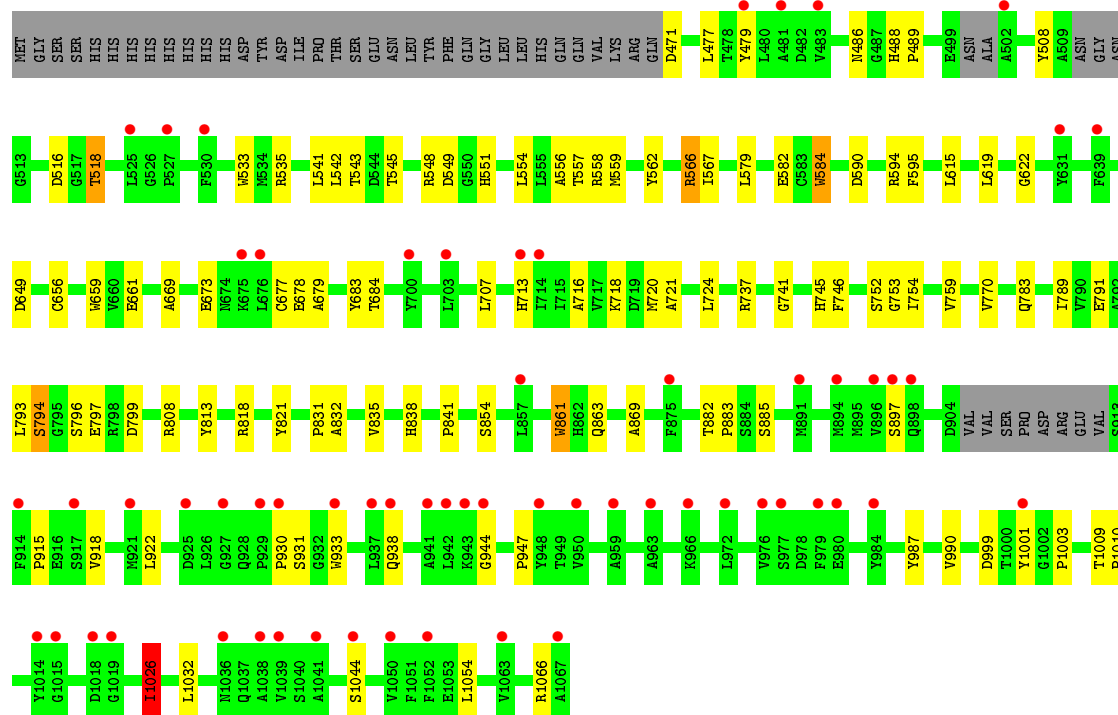
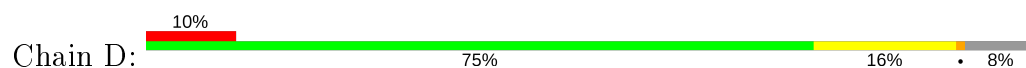
- Chain A:
-

- Chain B:
-
- 6% 81% 13% 6%

- Chain C:  8% 77% 14% 7%



• Molecule 1: Pyruvate carboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.81Å 157.28Å 245.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.78 48.22 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.78) 99.9 (48.22-2.78)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.01 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.209 , 0.258 0.211 , 0.259	Depositor DCC
R_{free} test set	4189 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	61.2	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17344	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, GOL, MG, PYR, KCX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.64	3/4542 (0.1%)	0.73	0/6192
1	B	0.55	4/4420 (0.1%)	0.67	1/6040 (0.0%)
1	C	0.59	3/4329 (0.1%)	0.69	0/5919
1	D	0.52	5/4292 (0.1%)	0.61	0/5872
All	All	0.58	15/17583 (0.1%)	0.68	1/24023 (0.0%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	659	TRP	CD2-CE2	6.77	1.49	1.41
1	C	659	TRP	CD2-CE2	5.94	1.48	1.41
1	D	659	TRP	CD2-CE2	5.48	1.48	1.41
1	D	584	TRP	CD2-CE2	5.46	1.47	1.41
1	B	533	TRP	CD2-CE2	5.44	1.47	1.41
1	B	601	TRP	CD2-CE2	5.31	1.47	1.41
1	D	533	TRP	CD2-CE2	5.21	1.47	1.41
1	D	861	TRP	CD2-CE2	5.20	1.47	1.41
1	D	933	TRP	CD2-CE2	5.14	1.47	1.41
1	A	861	TRP	CD2-CE2	5.13	1.47	1.41
1	C	601	TRP	CD2-CE2	5.07	1.47	1.41
1	A	533	TRP	CD2-CE2	5.04	1.47	1.41
1	B	659	TRP	CD2-CE2	5.03	1.47	1.41
1	C	933	TRP	CD2-CE2	5.03	1.47	1.41
1	B	861	TRP	CD2-CE2	5.01	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	476	LEU	CB-CG-CD1	-5.50	101.65	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4456	0	4275	27	0
1	B	4342	0	4039	47	0
1	C	4247	0	3885	55	0
1	D	4213	0	3832	62	0
2	A	6	0	3	0	0
2	B	6	0	3	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	C	6	0	8	3	0
6	A	28	0	0	0	0
6	B	12	0	0	3	0
6	C	12	0	0	0	0
6	D	8	0	0	0	0
All	All	17344	0	16045	185	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (185) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:677:CYS:H	1:D:713:HIS:CD2	1.81	0.97
1:C:883:PRO:HG2	1:C:926:LEU:HD21	1.45	0.95
1:C:566:ARG:HH11	1:C:566:ARG:CG	1.80	0.93
1:D:677:CYS:H	1:D:713:HIS:HD2	0.94	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:677:CYS:H	1:C:713:HIS:HD2	1.16	0.91
1:A:891[B]:MET:CE	1:A:918:VAL:HG21	2.01	0.89
1:C:566:ARG:HH11	1:C:566:ARG:HG2	1.35	0.89
1:A:891[B]:MET:HE3	1:A:918:VAL:HG21	1.59	0.84
1:D:793:LEU:O	1:D:796:SER:HB3	1.82	0.79
1:C:790:VAL:HG13	1:C:800:PRO:HG2	1.64	0.78
1:D:619:LEU:HD11	1:D:718:KCX:HE2	1.71	0.73
1:D:677:CYS:N	1:D:713:HIS:HD2	1.78	0.72
1:C:566:ARG:NH1	1:C:566:ARG:HG2	1.97	0.70
1:C:679:ALA:HB1	1:C:707:LEU:HD13	1.74	0.69
1:C:562:TYR:O	1:C:566:ARG:HG3	1.93	0.68
1:C:677:CYS:H	1:C:713:HIS:CD2	2.06	0.68
1:B:764:GLU:OE1	1:B:764:GLU:HA	1.93	0.68
1:A:953:GLY:HA2	1:A:956:LEU:HD12	1.74	0.68
1:B:938:GLN:HE22	1:B:947:PRO:HG3	1.58	0.67
1:B:482:ASP:OD2	1:B:1066:ARG:NH2	2.28	0.67
1:B:619:LEU:HD13	6:B:1211:HOH:O	1.94	0.67
1:D:549:ASP:HB3	1:D:783:GLN:HE22	1.63	0.64
1:C:520:GLN:O	1:C:524:THR:CG2	2.46	0.64
1:C:901:THR:O	1:C:904:ASP:HB2	1.97	0.63
1:C:664:ARG:HH21	1:C:710:ALA:HA	1.62	0.63
1:A:780:ASN:H	5:C:1101:GOL:H12	1.64	0.62
1:D:548:ARG:HB3	1:D:582:GLU:OE1	2.00	0.62
1:C:629:THR:OG1	1:C:630:ASN:N	2.32	0.61
1:D:679:ALA:HB1	1:D:707:LEU:HD22	1.81	0.61
1:C:621:ARG:O	1:C:623:ALA:N	2.34	0.61
1:D:486:ASN:HD21	1:D:1066:ARG:H	1.49	0.61
1:B:1043:ASP:C	1:B:1043:ASP:OD1	2.39	0.61
1:B:756:ALA:CB	1:D:754:ILE:HG22	2.32	0.60
1:C:928:GLN:NE2	1:C:949:THR:HA	2.17	0.59
1:B:1026:ILE:HG12	1:B:1032:LEU:CD1	2.32	0.59
1:D:558:ARG:O	1:D:821:TYR:HE1	1.86	0.59
1:D:535:ARG:HD3	1:D:741:GLY:O	2.02	0.59
1:A:891[B]:MET:HE2	1:A:891[B]:MET:HA	1.85	0.58
1:C:679:ALA:CB	1:C:707:LEU:HD13	2.32	0.58
1:A:555:LEU:HD11	1:A:818:ARG:HG3	1.85	0.58
1:B:486:ASN:ND2	1:B:1066:ARG:H	2.01	0.58
1:D:566:ARG:CG	1:D:566:ARG:HH11	2.16	0.57
1:B:844:GLN:HG2	1:B:844:GLN:O	2.03	0.57
1:B:567:ILE:HD13	1:B:813:TYR:CD2	2.40	0.56
1:C:566:ARG:HH11	1:C:566:ARG:HG3	1.65	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:ASP:OD1	1:A:800:PRO:HD2	2.06	0.56
1:D:543:THR:HG1	1:D:745:HIS:CE1	2.24	0.56
1:B:1026:ILE:HG12	1:B:1032:LEU:HD11	1.87	0.55
1:C:597:THR:HB	1:C:1004:VAL:HG21	1.89	0.55
1:A:778:SER:OG	1:C:831:PRO:HG2	2.07	0.55
1:C:664:ARG:NH2	1:C:710:ALA:HA	2.22	0.55
1:C:520:GLN:O	1:C:524:THR:HG23	2.06	0.54
1:B:836:TYR:CD2	1:D:791:GLU:HG2	2.42	0.54
1:B:744:ILE:HG13	6:B:1207:HOH:O	2.07	0.54
1:B:922:LEU:HB3	1:B:938:GLN:HG3	1.90	0.53
1:D:488:HIS:ND1	1:D:489:PRO:HD2	2.23	0.53
1:B:915:PRO:HB2	1:B:918:VAL:HG23	1.90	0.53
1:D:938:GLN:NE2	1:D:947:PRO:HB3	2.24	0.53
1:D:518:THR:HB	1:D:615:LEU:HG	1.92	0.52
1:B:720:MET:HG3	1:B:881:VAL:HG23	1.92	0.52
1:C:549:ASP:HB3	1:C:783:GLN:HE22	1.74	0.52
1:C:554:LEU:HD12	1:C:777:LEU:HD23	1.92	0.52
1:A:919:VAL:HG13	1:A:942:LEU:HD23	1.91	0.52
1:A:633:ASP:OD1	1:A:665:VAL:HG21	2.09	0.52
1:B:535:ARG:HD3	1:B:741:GLY:O	2.09	0.52
1:A:750:ASP:OD2	5:C:1101:GOL:O1	2.26	0.52
1:C:618:MET:HB3	1:C:648:ILE:HD12	1.92	0.52
1:B:494:ARG:HD2	1:B:823:ALA:O	2.09	0.51
1:C:520:GLN:O	1:C:524:THR:HG22	2.09	0.51
1:D:479:TYR:HB2	1:D:1001:TYR:HB3	1.92	0.51
1:C:1021:GLU:CG	1:C:1035:VAL:HG22	2.41	0.51
1:D:615:LEU:HA	1:D:649:ASP:OD2	2.11	0.51
1:A:549:ASP:HB3	1:A:783:GLN:HE22	1.76	0.51
1:A:907:SER:O	1:A:940:LYS:NZ	2.37	0.50
1:B:535:ARG:HD2	1:B:737:ARG:NH1	2.27	0.50
1:C:660:VAL:HG13	1:C:707:LEU:HD23	1.93	0.50
1:B:621:ARG:HB2	1:B:624:ASN:HB2	1.93	0.49
1:D:753:GLY:HA3	1:D:831:PRO:HB3	1.94	0.49
1:B:632:PRO:HB3	1:B:958:GLU:HA	1.93	0.49
1:C:539:ARG:HG3	1:C:539:ARG:O	2.12	0.49
1:D:566:ARG:CG	1:D:566:ARG:NH1	2.74	0.49
1:B:697:LEU:HD11	1:B:735:ALA:CB	2.43	0.49
1:D:683:TYR:CE1	1:D:724:LEU:HD13	2.48	0.49
1:C:987:TYR:HB3	1:C:990:VAL:HB	1.94	0.48
1:D:542:LEU:HD13	1:D:770:VAL:HG23	1.95	0.48
1:D:554:LEU:HD13	1:D:818:ARG:HH21	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:545:THR:HA	1:D:582:GLU:HB3	1.96	0.48
1:A:987:TYR:HB3	1:A:990:VAL:HB	1.93	0.48
1:B:835:VAL:HA	1:B:838:HIS:CE1	2.49	0.48
1:B:744:ILE:CG1	6:B:1207:HOH:O	2.60	0.48
1:B:965:ARG:NH2	1:B:976:VAL:O	2.47	0.47
1:C:661:GLU:HA	1:C:664:ARG:HG3	1.96	0.47
1:A:753:GLY:HA3	1:A:831:PRO:HB3	1.96	0.47
1:D:535:ARG:HH22	1:D:737:ARG:HB3	1.80	0.47
1:A:1025:ASP:OD2	1:A:1031:THR:OG1	2.26	0.47
1:B:753:GLY:HA3	1:B:831:PRO:HB3	1.96	0.47
1:D:562:TYR:O	1:D:566:ARG:HG3	2.15	0.47
1:D:615:LEU:HD22	1:D:649:ASP:HB3	1.97	0.47
1:A:537:GLU:HG3	1:A:539:ARG:HG2	1.97	0.46
1:C:1021:GLU:HG2	1:C:1035:VAL:HG22	1.96	0.46
1:C:615:LEU:HD22	1:C:649:ASP:HB3	1.96	0.46
1:D:656:CYS:SG	1:D:883:PRO:HD2	2.56	0.46
1:C:655:ASP:HB2	1:C:663:MET:HG2	1.97	0.46
1:A:887:VAL:HG13	1:A:918:VAL:HA	1.97	0.46
1:B:551:HIS:CE1	1:B:559:MET:HB3	2.51	0.46
1:D:566:ARG:HH11	1:D:566:ARG:HG3	1.79	0.46
1:D:594:ARG:HD3	1:D:595:PHE:CE2	2.50	0.46
1:B:1026:ILE:HA	1:B:1026:ILE:HD13	1.58	0.46
1:D:1026:ILE:HD11	1:D:1032:LEU:CG	2.45	0.46
1:D:922:LEU:O	1:D:938:GLN:NE2	2.49	0.46
1:A:520:GLN:O	1:A:524:THR:HG23	2.16	0.46
1:D:558:ARG:NH1	1:D:595:PHE:CD2	2.84	0.46
1:B:874:MET:C	1:B:876:GLY:H	2.20	0.45
1:D:549:ASP:HB3	1:D:783:GLN:NE2	2.30	0.45
1:D:752:SER:HB2	1:D:754:ILE:HG12	1.99	0.45
1:D:619:LEU:HD11	1:D:718:KCX:CE	2.45	0.45
1:D:838:HIS:HA	1:D:869:ALA:HB2	1.99	0.45
1:A:599:ASP:OD1	1:A:601:TRP:N	2.48	0.45
1:A:786:LEU:O	1:A:790:VAL:HG23	2.16	0.45
1:A:715:ILE:HB	1:A:744:ILE:HD13	1.98	0.45
1:D:549:ASP:HB2	1:D:582:GLU:OE1	2.17	0.45
1:D:861:TRP:O	1:D:861:TRP:CG	2.70	0.45
1:D:746:PHE:HB3	1:D:770:VAL:HG12	1.99	0.44
1:C:716:ALA:HA	1:C:745:HIS:O	2.17	0.44
1:D:678:GLU:OE2	1:D:716:ALA:HB2	2.17	0.44
1:D:759:VAL:HG11	1:D:789:ILE:HD13	2.00	0.44
1:C:678:GLU:OE1	1:C:745:HIS:ND1	2.44	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:837:LEU:HD21	1:B:866:GLN:OE1	2.18	0.44
1:C:655:ASP:OD1	1:C:662:ASN:HB3	2.18	0.44
1:B:541:LEU:HB3	1:B:579:LEU:HB2	1.99	0.44
1:C:676:LEU:HD22	1:C:714:ILE:HD11	1.99	0.44
1:D:915:PRO:HD2	1:D:918:VAL:HB	1.99	0.44
1:C:541:LEU:O	1:C:769:ALA:HA	2.18	0.43
1:C:627:GLY:HA3	1:C:631:TYR:HE2	1.83	0.43
1:B:987:TYR:HB3	1:B:990:VAL:HB	2.00	0.43
1:A:541:LEU:O	1:A:769:ALA:HA	2.17	0.43
1:B:667:MET:HG2	1:B:677:CYS:SG	2.58	0.43
1:D:554:LEU:HD13	1:D:818:ARG:NH2	2.32	0.43
1:B:485:VAL:HG12	1:B:486:ASN:ND2	2.34	0.43
1:B:525:LEU:O	1:B:529:LYS:HB2	2.18	0.43
1:C:584:TRP:HB3	1:C:618:MET:HB2	2.01	0.43
1:C:692:ARG:HH22	1:C:839:GLU:CD	2.22	0.43
1:B:482:ASP:CG	1:B:1066:ARG:HH21	2.21	0.43
1:B:812:PHE:CD1	1:B:812:PHE:N	2.86	0.43
1:C:951:ARG:HA	1:C:952:PRO:HD3	1.76	0.43
1:B:963:ALA:O	1:B:967:VAL:HG23	2.18	0.43
1:C:476:LEU:O	1:C:479:TYR:N	2.52	0.43
1:C:926:LEU:HA	1:C:926:LEU:HD12	1.74	0.43
1:D:558:ARG:O	1:D:821:TYR:CE1	2.68	0.43
1:B:766:GLY:HA2	1:B:798:ARG:NH1	2.34	0.43
1:D:590:ASP:HB2	1:D:987:TYR:CZ	2.53	0.43
1:D:567:ILE:HB	1:D:813:TYR:CE2	2.54	0.42
1:B:535:ARG:CZ	1:B:737:ARG:HD3	2.49	0.42
1:B:669:ALA:O	1:B:673:GLU:HG2	2.19	0.42
1:C:477:LEU:HD11	1:C:1054:LEU:HD22	2.01	0.42
1:D:794:SER:HA	1:D:799:ASP:OD2	2.19	0.42
1:C:793:LEU:HD23	1:C:793:LEU:HA	1.76	0.42
1:B:603:ARG:O	1:B:607:ILE:HG13	2.19	0.42
1:C:743:PRO:HA	1:C:768:ASP:OD2	2.20	0.42
1:B:486:ASN:HD21	1:B:1066:ARG:H	1.68	0.42
1:D:486:ASN:ND2	1:D:1066:ARG:H	2.14	0.42
1:D:987:TYR:HB3	1:D:990:VAL:HB	2.00	0.41
1:D:721:ALA:HA	1:D:841:PRO:HA	2.01	0.41
1:D:541:LEU:HB3	1:D:579:LEU:HB2	2.02	0.41
1:B:834:GLU:HA	1:D:808:ARG:HD2	2.03	0.41
1:B:477:LEU:HD11	1:B:1054:LEU:HD22	2.03	0.41
1:C:981:PHE:O	1:C:985:LEU:HG	2.21	0.41
1:C:750:ASP:OD2	5:C:1101:GOL:C3	2.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1009:THR:HB	1:D:1010:PRO:HD3	2.03	0.41
1:A:540:VAL:HG21	1:A:763:VAL:HG22	2.03	0.41
1:C:535:ARG:HD3	1:C:741:GLY:O	2.21	0.41
1:A:756:ALA:CB	1:C:754:ILE:HG22	2.51	0.41
1:B:1043:ASP:OD1	1:B:1045:GLN:N	2.54	0.41
1:B:756:ALA:HB1	1:D:754:ILE:HG22	2.03	0.41
1:D:832:ALA:O	1:D:835:VAL:HG12	2.21	0.41
1:A:928:GLN:HA	1:A:929:PRO:HD3	1.88	0.40
1:C:656:CYS:HA	1:C:881:VAL:CG1	2.52	0.40
1:D:556:ALA:O	1:D:558:ARG:HD3	2.22	0.40
1:A:894:MET:HE1	1:A:915:PRO:HD3	2.02	0.40
1:C:753:GLY:HA3	1:C:831:PRO:HB3	2.03	0.40
1:C:872:ASN:O	1:C:876:GLY:O	2.39	0.40
1:D:477:LEU:HD11	1:D:1054:LEU:HD22	2.02	0.40
1:C:901:THR:N	1:C:904:ASP:HB2	2.36	0.40
1:D:551:HIS:CG	1:D:559:MET:HB2	2.56	0.40
1:D:669:ALA:O	1:D:673:GLU:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	591/632 (94%)	563 (95%)	27 (5%)	1 (0%)	47	76
1	B	586/632 (93%)	549 (94%)	35 (6%)	2 (0%)	41	70
1	C	582/632 (92%)	533 (92%)	44 (8%)	5 (1%)	17	44
1	D	575/632 (91%)	542 (94%)	27 (5%)	6 (1%)	15	41
All	All	2334/2528 (92%)	2187 (94%)	133 (6%)	14 (1%)	25	54

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	501	ALA
1	C	622	GLY
1	C	943	LYS
1	D	622	GLY
1	B	908	PRO
1	C	1041	ALA
1	C	1055	ASN
1	D	508	TYR
1	D	944	GLY
1	A	500	ASN
1	D	1026	ILE
1	D	930	PRO
1	C	492	LYS
1	D	1003	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	443/518 (86%)	425 (96%)	18 (4%)	30	61
1	B	419/518 (81%)	405 (97%)	14 (3%)	38	69
1	C	394/518 (76%)	367 (93%)	27 (7%)	15	38
1	D	395/518 (76%)	375 (95%)	20 (5%)	24	53
All	All	1651/2072 (80%)	1572 (95%)	79 (5%)	25	55

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	524	THR
1	A	557	THR
1	A	584	TRP
1	A	594	ARG
1	A	597	THR
1	A	633	ASP
1	A	720	MET
1	A	754	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	854	SER
1	A	882	THR
1	A	897	SER
1	A	899	ASP
1	A	911	GLU
1	A	917	SER
1	A	935	GLU
1	A	950	VAL
1	A	1008	PRO
1	A	1016	LEU
1	B	584	TRP
1	B	692	ARG
1	B	720	MET
1	B	737	ARG
1	B	752	SER
1	B	791	GLU
1	B	826	SER
1	B	855	LEU
1	B	882	THR
1	B	901	THR
1	B	926	LEU
1	B	975	GLU
1	B	998	SER
1	B	1026	ILE
1	C	510	ASN
1	C	521	LEU
1	C	524	THR
1	C	546	THR
1	C	553	SER
1	C	557	THR
1	C	566	ARG
1	C	577	ASN
1	C	584	TRP
1	C	597	THR
1	C	629	THR
1	C	661	GLU
1	C	664	ARG
1	C	689	ASN
1	C	699	TYR
1	C	720	MET
1	C	767	VAL
1	C	777	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	794	SER
1	C	848	LEU
1	C	882	THR
1	C	899	ASP
1	C	951	ARG
1	C	1005	SER
1	C	1021	GLU
1	C	1025	ASP
1	C	1047	MET
1	D	471	ASP
1	D	516	ASP
1	D	518	THR
1	D	557	THR
1	D	566	ARG
1	D	584	TRP
1	D	661	GLU
1	D	684	THR
1	D	720	MET
1	D	794	SER
1	D	797	GLU
1	D	854	SER
1	D	863	GLN
1	D	882	THR
1	D	885	SER
1	D	897	SER
1	D	931	SER
1	D	999	ASP
1	D	1026	ILE
1	D	1044	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	486	ASN
1	A	630	ASN
1	A	783	GLN
1	B	486	ASN
1	B	630	ASN
1	B	783	GLN
1	B	938	GLN
1	C	630	ASN
1	C	689	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	713	HIS
1	C	783	GLN
1	C	866	GLN
1	D	486	ASN
1	D	630	ASN
1	D	713	HIS
1	D	783	GLN
1	D	938	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	KCX	C	718	1,3	7,11,12	0.61	0	4,12,14	1.06	0
1	KCX	D	718	1,3	7,11,12	0.63	0	4,12,14	1.81	2 (50%)
1	KCX	A	718	1,3	7,11,12	0.69	0	4,12,14	4.42	2 (50%)
1	KCX	B	718	1,3	7,11,12	0.64	0	4,12,14	1.27	1 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	C	718	1,3	-	4/7/10/12	-
1	KCX	D	718	1,3	-	5/7/10/12	-
1	KCX	A	718	1,3	-	5/7/10/12	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	B	718	1,3	-	1/7/10/12	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	718	KCX	CE-NZ-CX	7.95	136.41	122.95
1	A	718	KCX	CD-CE-NZ	3.84	121.81	111.49
1	D	718	KCX	CE-NZ-CX	2.46	127.12	122.95
1	D	718	KCX	CD-CE-NZ	2.34	117.79	111.49
1	B	718	KCX	CE-NZ-CX	2.26	126.78	122.95

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	718	KCX	N-CA-CB-CG
1	C	718	KCX	C-CA-CB-CG
1	C	718	KCX	O-C-CA-CB
1	D	718	KCX	O-C-CA-CB
1	D	718	KCX	CD-CE-NZ-CX
1	A	718	KCX	O-C-CA-CB
1	A	718	KCX	CD-CE-NZ-CX
1	B	718	KCX	O-C-CA-CB
1	A	718	KCX	CG-CD-CE-NZ
1	D	718	KCX	CG-CD-CE-NZ
1	A	718	KCX	CA-CB-CG-CD
1	A	718	KCX	C-CA-CB-CG
1	C	718	KCX	CE-CD-CG-CB
1	D	718	KCX	CE-CD-CG-CB
1	D	718	KCX	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	718	KCX	2	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GOL	C	1101	-	5,5,5	0.36	0	5,5,5	1.39	1 (20%)
2	PYR	B	1101	-	2,5,5	0.32	0	2,6,6	0.27	0
2	PYR	A	1101	-	2,5,5	0.27	0	2,6,6	0.16	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	C	1101	-	-	0/4/4/4	-
2	PYR	B	1101	-	-	0/0/4/4	-
2	PYR	A	1101	-	-	0/0/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1101	GOL	C3-C2-C1	-2.07	103.67	111.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1101	GOL	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	594/632 (93%)	-0.17	7 (1%) 79 76	32, 51, 74, 124	18 (3%)
1	B	592/632 (93%)	0.20	39 (6%) 18 13	40, 71, 138, 196	19 (3%)
1	C	587/632 (92%)	0.39	52 (8%) 9 6	33, 83, 158, 199	15 (2%)
1	D	583/632 (92%)	0.47	61 (10%) 6 4	58, 89, 126, 147	15 (2%)
All	All	2356/2528 (93%)	0.22	159 (6%) 17 13	32, 71, 136, 199	67 (2%)

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	934	PRO	6.8
1	D	914	PHE	5.9
1	C	936	ALA	5.2
1	C	937	LEU	4.8
1	D	713	HIS	4.6
1	B	909	ASP	4.5
1	C	940	LYS	4.4
1	C	981	PHE	4.4
1	C	876	GLY	4.4
1	D	896	VAL	4.3
1	D	891	MET	4.3
1	C	933	TRP	4.2
1	B	872	ASN	4.1
1	B	874	MET	4.1
1	D	941	ALA	4.1
1	D	525	LEU	4.0
1	B	941	ALA	4.0
1	C	893	LEU	3.9
1	B	963	ALA	3.9
1	B	878	ILE	3.9
1	B	902	VAL	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	875	PHE	3.8
1	D	676	LEU	3.8
1	B	934	PRO	3.8
1	D	479	TYR	3.8
1	B	700	TYR	3.7
1	C	1048	VAL	3.7
1	D	937	LEU	3.7
1	C	874	MET	3.7
1	D	963	ALA	3.6
1	C	1039	VAL	3.6
1	B	908	PRO	3.6
1	D	483	VAL	3.5
1	B	961	LEU	3.5
1	D	639	PHE	3.5
1	B	933	TRP	3.4
1	B	900	LEU	3.4
1	B	891	MET	3.4
1	C	1016	LEU	3.4
1	D	950	VAL	3.4
1	D	938	GLN	3.4
1	B	936	ALA	3.3
1	C	894	MET	3.3
1	D	942	LEU	3.3
1	C	659	TRP	3.3
1	C	891	MET	3.3
1	D	897	SER	3.2
1	C	976	VAL	3.2
1	B	876	GLY	3.2
1	C	906	VAL	3.2
1	C	1063	VAL	3.2
1	D	1067	ALA	3.2
1	D	894	MET	3.2
1	D	1039	VAL	3.2
1	D	930	PRO	3.1
1	D	1018	ASP	3.1
1	D	944	GLY	3.1
1	C	510	ASN	3.1
1	D	943	LYS	3.0
1	D	976	VAL	3.0
1	C	938	GLN	3.0
1	B	830	GLY	3.0
1	B	864	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	966	LYS	3.0
1	C	1047	MET	3.0
1	D	631	TYR	2.9
1	B	906	VAL	2.9
1	C	622	GLY	2.9
1	B	937	LEU	2.9
1	D	948	TYR	2.9
1	B	893	LEU	2.9
1	D	917	SER	2.8
1	C	875	PHE	2.8
1	D	927	GLY	2.8
1	D	1036	ASN	2.8
1	D	1044	SER	2.8
1	C	782	SER	2.7
1	C	479	TYR	2.7
1	D	857	LEU	2.7
1	D	898	GLN	2.7
1	C	502	ALA	2.7
1	D	703	LEU	2.7
1	D	502	ALA	2.7
1	C	753	GLY	2.7
1	A	512	ASN	2.7
1	C	963	ALA	2.7
1	D	1038	ALA	2.7
1	D	714	ILE	2.6
1	D	925	ASP	2.6
1	C	1050	VAL	2.6
1	B	965	ARG	2.6
1	A	968	ILE	2.6
1	D	984	TYR	2.6
1	B	912	VAL	2.6
1	D	972	LEU	2.6
1	D	1015	GLY	2.6
1	D	1041	ALA	2.6
1	D	1063	VAL	2.6
1	C	941	ALA	2.6
1	D	933	TRP	2.6
1	D	700	TYR	2.5
1	D	1014	TYR	2.5
1	C	1049	THR	2.5
1	C	932	GLY	2.5
1	D	977	SER	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	1052	PHE	2.5
1	D	1001	TYR	2.5
1	C	897	SER	2.5
1	A	779	GLY	2.5
1	C	904	ASP	2.4
1	D	980	GLU	2.4
1	B	892	ALA	2.4
1	C	485	VAL	2.4
1	D	530	PHE	2.4
1	C	930	PRO	2.4
1	B	863	GLN	2.4
1	C	781	THR	2.4
1	B	877	ASP	2.4
1	C	872	ASN	2.4
1	B	875	PHE	2.3
1	C	483	VAL	2.3
1	C	546	THR	2.3
1	D	979	PHE	2.3
1	A	961	LEU	2.3
1	C	487	GLY	2.3
1	B	992	THR	2.3
1	D	1019	GLY	2.3
1	B	750	ASP	2.3
1	C	831	PRO	2.2
1	B	968	ILE	2.2
1	B	913	SER	2.2
1	D	959	ALA	2.2
1	B	962	ASP	2.2
1	B	635	VAL	2.2
1	B	501	ALA	2.2
1	D	921	MET	2.2
1	B	751	THR	2.2
1	D	527	PRO	2.2
1	D	675	LYS	2.2
1	A	750	ASP	2.2
1	C	830	GLY	2.2
1	D	481	ALA	2.2
1	B	907	SER	2.2
1	A	778	SER	2.1
1	C	975	GLU	2.1
1	C	780	ASN	2.1
1	A	751	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	942	LEU	2.1
1	C	944	GLY	2.1
1	D	1050	VAL	2.1
1	C	867	ALA	2.1
1	C	476	LEU	2.0
1	B	754	ILE	2.0
1	D	929	PRO	2.0
1	C	557	THR	2.0
1	C	919	VAL	2.0
1	B	938	GLN	2.0
1	B	873	GLN	2.0
1	C	553	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	KCX	D	718	12/13	0.95	0.19	73,77,87,90	0
1	KCX	C	718	12/13	0.96	0.19	64,67,76,77	0
1	KCX	B	718	12/13	0.97	0.19	68,71,78,81	0
1	KCX	A	718	12/13	0.98	0.21	40,42,58,59	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	D	1102	1/1	0.76	0.07	75,75,75,75	0
4	MG	A	1103	1/1	0.88	0.11	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PYR	B	1101	6/6	0.90	0.25	74,80,88,91	0
4	MG	C	1103	1/1	0.91	0.10	55,55,55,55	0
5	GOL	C	1101	6/6	0.92	0.81	22,24,24,25	6
2	PYR	A	1101	6/6	0.94	0.31	24,26,26,27	6
3	ZN	D	1101	1/1	0.96	0.12	77,77,77,77	0
3	ZN	C	1102	1/1	0.97	0.16	72,72,72,72	0
3	ZN	B	1102	1/1	0.98	0.11	78,78,78,78	0
3	ZN	A	1102	1/1	0.99	0.15	58,58,58,58	0
4	MG	B	1103	1/1	0.99	0.08	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.